# Table of Contents

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2. Daily Schedule
8. Tutorials | BOFs
9. Visualization Showcase
   Special Presentations
10. Posters and Demos
11. Student Posters
12. Sponsors
13. Floor Plan
**Dr. Gabrielle Allen | Tuesday August 3rd, 9:00 am**
Accurately modeling astrophysical systems that are governed by Einstein’s Equations of General Relativity, such as black holes, stellar core collapse, or gamma ray bursts, require the use of cutting edge computational resources and software. In this talk, Dr. Allen will describe how numerical relativity has motivated and led to the development of the Cactus Framework - an open, collaborative component framework and set of toolkits for scientific computing, as well as numerous advanced scenarios exploiting Grid and distributed computing, high-speed networks, and advanced visualization. She will describe how this work has led to a new software effort in numerical relativity, the Einstein Toolkit Consortium, which is developing and supporting the software for state-of-the-art simulations involving general relativistic “magnetohydrodynamics” and working toward a sustainable model for software development. Finally, Dr. Allen will discuss the importance of the TeraGrid and prior national resources in supporting these and reflect on current and future needs in scientific computing infrastructure.

**Dr. Tim Killeen | Wednesday August 4th, 8:45 am**
The NSF Geosciences Directorate has long supported the development of sustained cyberinfrastructure. These investments have significantly increased the capabilities and productivity of the national geosciences community. Complementary investments made by other directorates and offices within NSF, and by other agencies, have enhanced and leveraged the GEO-funded programs. As a result, a rich portfolio of cyberinfrastructure tools and capabilities, together with an experienced and knowledgeable community has resulted. The Geosciences community has worked with systems that encompass, for example, workstations to supercomputers, smart sensors to global remote sensor networks, and sophisticated data systems available to large communities of users. Also, programs to develop human capital have been emphasized, ranging from graduate student educational programs to post-docs cyberinfrastructure programs and support for technology leaders for the entire science community. On the horizon is yet another round of investments that will provide the geosciences community with an ever-expanding range of capabilities for discovery. Dr. Killeen will present a brief review of the geosciences investments in cyberinfrastructure and some of the significant outcomes and future plans.

**Dr. Bob Wilhelmson | Thursday August 5th, 9:15 am**
Blue Waters is expected to be the most powerful supercomputer in the world for open scientific research when it comes online in 2011. The system is a joint effort between NCSA, the University of Illinois, IBM, and the National Science foundation. It will be the first system of its kind to sustain one petaflop performance on a range of science and engineering applications. The project includes provision of the computer system and intense collaboration with dozens of teams in the development of science and engineering applications. This collaboration will help ensure that scientists and engineers across the country will be able to use Blue Waters to its fullest potential. Dr. Wilhelmson will provide a brief overview of the Blue Waters project and focus on some of the applications that are being prepared for use on the system when it becomes available.
On-site registration will be in the Lobby at the following times:
Sunday, August 1: 4 pm – 7 pm  |  Monday, August 2: 7 am – 5 pm  |  Tuesday, August 3: 7:30 am – 5 pm

STUDENT RECEPTION: Sunday, August 1: 7 pm – 9 pm [Fountain View]

<table>
<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Event</th>
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<tbody>
<tr>
<td>7:00 am - 8:00 am</td>
<td>Admiral Room</td>
<td>CONTINENTAL BREAKFAST</td>
</tr>
<tr>
<td>8:00 am - 5:00 pm</td>
<td>Waterfront, Brighton III &amp; IV</td>
<td>How to design a cluster that works with the TG (Pt 1)</td>
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<tr>
<td></td>
<td>Grand Station III</td>
<td>Introduction to scientific visualization on Longhorn (Pt 1)</td>
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<td></td>
<td>Grand Station IV</td>
<td>Running applications at scale on the first academic petaflop supercomputer (Pt 1)</td>
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<td></td>
<td>Grand Station V</td>
<td>Cloud technologies, data-intensive science and the TG (Pt 1)</td>
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<td></td>
<td>Ellwood</td>
<td>Building Science Gateway Applications (Pt 1)</td>
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<td></td>
<td>Haselton</td>
<td>HPC Applications Best Practices (Pt 1)</td>
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<tr>
<td></td>
<td>Brighton I</td>
<td>Optimization in multi-core systems (Pt 1)</td>
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<td></td>
<td>Brighton II</td>
<td>Parallel simulations &amp; Science Gateways on the MATLAB Resource at Cornell (Pt 1)</td>
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<tr>
<td>10:00 am - 10:30 am</td>
<td>Grand Ballrooms</td>
<td>BREAK</td>
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<tr>
<td>10:30 am - 12:00 pm</td>
<td>Grand Station II</td>
<td>How to design a cluster that works with the TG (Pt 2)</td>
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<td>Brighton II</td>
<td>Parallel simulations &amp; Science Gateways on the MATLAB Resource at Cornell (Pt 2)</td>
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<tr>
<td>12:00 pm - 1:00 pm</td>
<td>Admiral Room</td>
<td>LUNCH</td>
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<tr>
<td>1:00 pm - 2:15 pm</td>
<td>Grand Station II</td>
<td>Computing across Open Science Grid and TG (Pt 1)</td>
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<td>Grand Station III</td>
<td>Introducing RDAV &amp; Nautilus for visualization, data analysis and workflows (Pt 1)</td>
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<td>Grand Station IV</td>
<td>Running applications at scale on the first academic petaflop supercomputer (Pt 3)</td>
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<td>Grand Station V</td>
<td>Open grid environments software for Science Gateways (Pt 1)</td>
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<td></td>
<td>Ellwood</td>
<td>Performance Analysis and Tuning for GPUs (Pt 1)</td>
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<td>Haselton</td>
<td>PerfExpert: Automated Approach to Analyzing &amp; Optimizing the Node-Level Performance of HPCApps (Pt 1)</td>
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<td>Brighton I</td>
<td>vSMP and Flash technologies for data-intensive applications (Pt 1)</td>
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<td>Brighton II</td>
<td>Scalable systems management with Puppet (Pt 1)</td>
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<td>2:15 pm - 2:30 pm</td>
<td>Grand Ballrooms</td>
<td>BREAK</td>
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<td>Foyer</td>
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<td>2:30 pm - 5:00 pm</td>
<td>Grand Station II</td>
<td>Computing across Open Science Grid and TG (Pt 2)</td>
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<td>Brighton II</td>
<td>Scalable systems management with Puppet (Pt 2)</td>
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<tr>
<td>6:00 pm - 7:30 pm</td>
<td>Admiral, Waterfront, Reflections</td>
<td>CASUAL RECEPTION</td>
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<tr>
<td>Time</td>
<td>Location</td>
<td>Event Description</td>
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<tr>
<td>7:30 am - 8:30 am</td>
<td>Reflections, Waterfront</td>
<td><strong>BREAKFAST</strong></td>
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<tr>
<td>8:00 am - 5:00 pm</td>
<td>Haselton</td>
<td><strong>Students Programming Contest (All day event)</strong></td>
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</table>
| 8:15 am - 9:45 am  | Grand Station I-V               | Welcoming Remarks  
TG Overview  
Keynote: Gabrielle Allen (Louisiana State University, Computational Astrophysics) |
| 9:45 am - 10:00 am | Grand Ballrooms Foyer           | **BREAK**                                                                         |
| 10:00 am - 10:30 am| Grand Stations III & IV         | Science Track  
Session chair: Amit Majumdar, Jeff Gardner                                       |
| 10:03 am - 11:00 am| 3D Global Hybrid Simulations    | of the Magnetosphere and I/O Strategies for Massively Parallel Kinetic Simulations |
|                    |                                 | Homa Karimabadi                                                                   |
| 11:00 am - 11:30 am| High-throughput computing       | of large-scale ensembles on the TeraGrid and DEISA for HIV-I Protease Simulation  |
|                    |                                 | Shantenu Jha                                                                       |
| 11:30 am - 12:00 pm| Asynchronous Implementation of  | A Parallel Genetic Algorithm for the Generalized Assignment Problem               |
|                    |                                  | Yan Liu, Shaowen Wang                                                              |
| 12:00 pm - 1:15 pm | Reflections, Waterfront         | **LUNCH**                                                                         |
| 12:00 pm - 1:00 pm | Woodlawn I - Edenburg - Ellwood I - Ellwood II - Stoops Ferry | **Working Groups**  
Data  
EOT  
Common User  
Advanced User  
Visualization |
| 1:15 pm - 2:15 pm  | Grand Station I-II              | Panel Session Advanced Cyberinfrastructure Integration with Large Scale NSF Science and Engineering Projects  
Panelists: Kent Blackburn (LIGO), Barb Fossum (NEES), John Orcutt (OOI), Dan Stanzione (iPlant) |
| 2:15 pm - 2:30 pm  | Grand Ballrooms Foyer           | **BREAK**                                                                         |

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<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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| 2:30 pm-3:00 pm | Invited talk; Accelerating Data-Intensive Science with Gordon and Dash  
*Michael Norman, Allan Snavely*                                                                 |
| 3:00 pm-3:30 pm | Patterns in Bird Migration  
Phenology Explored through Data Intensive Computation  
*Steven Kelling, Daniel Fink, Robert Cook, Suresh Santhana Vannan, John Cobb, Kevin Webb, William Michener* |
| 3:30 pm-4:00 pm | A Compelling Case for a Centralized Filesystem on the TeraGrid: Enhancing an astrophysical workflow with the Data Capacitor WAN as a test case  
*Scott Michael, Stephen Simms, W. B. (Trey) Breckenridge, Roger Smith, Matthew Link* |
| 4:00 pm-4:15 pm | Break                                                                                                                   |
| 4:15 pm-4:45 pm | Cosmological structure formation at the largest and smallest scales  
*Brian O'Shea, Michael Norman, Jack Burns, Matthew Turk, Britton Smith, Sam Skillman, John Wise* |
| 4:45 pm-5:15 pm | Turbulence in Molecular Clouds: Inferences from Simulations of Multiphase Interstellar Medium  
*Alexei Kritsuk, Segrey Ustyugov, Michael Norman* |
| 5:15 pm-5:30 pm | Break                                                                                                                   |
| 5:30 pm-6:30 pm | Working Groups  
Software Allocations                                                                                                    |
| 5:30 pm-7:00 pm | BOFS  
New Compute Systems in the TeraGrid Pipeline (Pt I)  
"MATLAB on the TeraGrid" Experimental Resource: Information, Getting Started & Success Stories  
Data Curation and Management in the TeraGrid  
Extending Cyberinfrastructure Beyond Its Own Boundaries - Campus Champion Program |
| 7:00 pm-9:00 pm | VISUALIZATION GALLERY AND POSTER RECEPTION                                                                                 |
### Daily Schedule

**WEDNESDAY, AUGUST 4, 2010**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>7:30 am</td>
<td>Reflections, Waterfront</td>
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<tr>
<td>8:30 am</td>
<td><strong>Continental Breakfast</strong></td>
</tr>
<tr>
<td>9:45 am</td>
<td><strong>BREAK</strong></td>
</tr>
</tbody>
</table>
| 10:00 am - 10:30 am | Grand Stations III & IV  
  **Science Track**  
  Session chair: Philip Blood, Mahidhar Tatineni  
  Invited talk; Uintah a scalable framework for hazard analysis  
  Martin Berzins, Justin Luitjens, Qingyu Meng, Todd Harman, Charles Wight, Joseph Peterson |
| 10:30 am - 11:00 am | Grand Stations III & IV  
  **Technology Track**  
  Session chair: Warren Smith  
  Petascale I/O using HDF-5  
  Nicholas Malaya, Karl Schulz, Robert Moser  
  Modelling Data-driven CO2 Sequestration Using Distributed HPC Cyberinfrastructure  
  Yaakoub El Khamra, Shantenu Jha, Christopher White |
| 11:00 am - 11:30 am | Grand Stations III & IV  
  **Science Track**  
  Session chair: Philip Blood, Mahidhar Tatineni  
  Computational Explorations into the HINI Pandemic  
  Shawn Brown, Phil Cooley, Bruce Y. Lee, William Wheaton, John Grefenstette, Donald Burke |
| 11:30 am - 12:00 pm | Grand Stations III & IV  
  **Science Track**  
  Session chair: Philip Blood, Mahidhar Tatineni  
  Agent-based Modeling of Agricultural Land Use on TeraGrid  
  Anand Padmanabhan, Wenwu Tang, Shaowen Wang  
  **Technology Track**  
  Session chair: Warren Smith  
  Kerberized Lustre 2.0 over the WAN  
  Josephine Palencia, Robert Budden, Kevin Sullivan  
  DASH-IO: an Empirical Study of Flash-based IO for HPC  
  Jiahua He, Jeffrey Bennett, Allan Snively  
  **EOT Track**  
  Session chair: Scott McCaulay, Edee Wiziecki  
  Virtual Appliances for Training and Education in FutureGrid  
  Renato Figueiredo, Arjun Prakash, David Wolinsky |
| 12:00 pm - 1:15 pm | Grand Stations III & IV  
  **Science Track**  
  Session chair: Philip Blood, Mahidhar Tatineni  
  Agent-based Modeling of Agricultural Land Use on TeraGrid  
  Anand Padmanabhan, Wenwu Tang, Shaowen Wang  
  **Technology Track**  
  Session chair: Warren Smith  
  Enabling Lustre WAN for Production Use on the TeraGrid: A Lightweight UID Mapping Scheme  
  Stephen Simms, Joshua Wolgenbach, Justin Miller, Kit Westneat  
  **EOT Track**  
  Session chair: Scott McCaulay, Edee Wiziecki  
  A Desktop to TeraGrid Ecosystem  
  Jill Gemmill, Jim Bottum, Peter Cummings, Tom Finholt, Igor Joulina, Stephen Lanier, Ken Lewis, Nicholas Panasik, Jack Wells  
  Cyberinfrastructure Campus Bridging with Campus Champions  
  Dan Fraser, Kay Hunt, Scott Lathrop, Roger Moye, James Barr von Oehsen, Ruth Pordes, Jeff Pummill  
  A Vision for Cyberlearning and Workforce Development  
  Alex Ramirez, Diane Baxter, Scott Lathrop |
| 12:00 pm - 1:15 pm | Grand Station I-II  
  **Plenary Session:** Technology Audit and Insertion Services, and Sponsor Presentation (Dell) Tom Furlani, John Towns, and Jim Gutowski |
| 1:15 pm - 2:15 pm | **BREAK**                                                             |

**LUNCH**

**Working Groups**
- External Relations
- Network
- User Facing
- Science Gateways
- Q/A

**Continued...**
**WEDNESDAY, AUGUST 4, 2010 (cont’d)**

<table>
<thead>
<tr>
<th>Time</th>
<th>Grand Stations III &amp; IV</th>
<th>Brighton I-V</th>
<th>Reflections</th>
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</thead>
<tbody>
<tr>
<td>2:30 pm - 3:00 pm</td>
<td>Invited talk; Long-timescale simulations of GPCRs on Anton, a specialized molecular dynamics machine</td>
<td>Invited talk; Long-timescale simulations of GPCRs on Anton, a specialized molecular dynamics machine</td>
<td>Beowulf Bootcamp: Teaching Local High Schools about HPC</td>
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<td></td>
<td>Ron Dror</td>
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<td>Steven Brandt, Chirag Dekate, Philip LeBlanc, Thomas Sterling</td>
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<tr>
<td>3:00 pm - 3:30 pm</td>
<td>Acceleration of AMBER Molecular Dynamics Simulations using NVIDIA GPUs: Performance Improvements, Validation and Lessons Learned</td>
<td>Acceleration of AMBER Molecular Dynamics Simulations using NVIDIA GPUs: Performance Improvements, Validation and Lessons Learned</td>
<td>Not Stuck in the Shallow End but Riding the Wave of Opportunity in TeraGrid-Inspired Outreach</td>
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<td>Ross Walker</td>
<td></td>
<td>Bonnie Bracey Sutton, Vic Sutton</td>
</tr>
<tr>
<td>3:30 pm - 4:00 pm</td>
<td>A Novel Approach to Parallel 3-D FFT</td>
<td>ActionFolders: Automation, Notification, Workflow</td>
<td>Computation and Visualization for High School Chemistry Educators and Students at the Institute for Chemistry Literacy Through Computational Science (ICLCS)</td>
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<td>Yang Wang, Anthony Rollett</td>
<td>Ron Dooley, Maytal Dahan</td>
<td>Edee Wiziecki, R. Jay Mashl, Bernard A'cs, Michael Evans, Jeffrey Moore</td>
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<tr>
<td>4:00 pm - 4:15 pm</td>
<td>BREAK</td>
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<tr>
<td>4:15 pm - 4:45 pm</td>
<td>Biomolecular modeling using NAMD on TeraGrid machines</td>
<td>Design and Implementation of a Production Dynamically Configurable Testbed</td>
<td>Accelerating Science Gateway Development with Web 2.0 and Swift</td>
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<td>Abhinav Bhatere, Eric Lee, Ly Le, Leonardo Trabuco, Eduard Schreiner, Jen Hsin, James C. Phillips, Laxmikant V. Kale, Klaus Schulten</td>
<td>Kenny Welshons, Patrick Dorn, Andrei Hutana, Petr Halub, John Vollbrecht, Gabrielle Allen</td>
<td>Wenjun Wu, Thomas Uram, Michael Wilde, Mark Hered, Michael E. Papka</td>
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<tr>
<td>4:45 pm - 5:15 pm</td>
<td>BioDrugScreen: a computational drug design resource for ranking molecules docked to the human proteome</td>
<td>DataONE: Building a virtual data center for the biological, ecological and environmental sciences</td>
<td>Open Grids Computing Environments: Advanced Gatew-ay Support Activities</td>
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<td>Liwei Li, Khuchtumur Bum-Erdene, Josh Rosen, Marlon Pierce, Sammy Meroueh</td>
<td>William Michener, John Cobb, Robert Cook, Rebecca Koskela, Dave Viegla</td>
<td>Marlon Pierce, Suresh Marru, Raminder Singh, Archit Kulshrestha, Karthik Muthuraman</td>
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<tr>
<td>5:15 pm - 6:15 pm</td>
<td>Stoops Ferry, Ellwood I, Edenburg, Ellwood II</td>
<td>BOFS - New Compute Systems in the TeraGrid Pipeline (Part 2)</td>
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<tr>
<td>5:30 pm - 6:30 pm</td>
<td>Woodlawn I, Working Group Scheduling</td>
<td>Common User Environments Working Group - Progress Report of Users</td>
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<tr>
<td>7:00 pm - 10:00 pm</td>
<td>Station Square</td>
<td>NSF DataNet Program overview and community input solicitation</td>
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**Stoops Ferry**
- Ellwood I
- Edenburg
- Ellwood II

**BoFS**
- New Compute Systems in the TeraGrid Pipeline (Part 2)
- Common User Environments Working Group - Progress Report of Users
- NSF DataNet Program overview and community input solicitation
- SLASH2: Next Generation Filesystem for Cooperating Scientific Institutions

**DINNER CRUISE**
<table>
<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Event/Session</th>
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<tbody>
<tr>
<td>7:30 am</td>
<td>Waterfront</td>
<td>CONTINENTAL BREAKFAST</td>
</tr>
<tr>
<td>8:30 am</td>
<td>Grand Station I-V</td>
<td>Conference Awards</td>
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<tr>
<td>9:15 am</td>
<td>Grand Station I-V</td>
<td>Keynote: Bob Wilhelmson (National Center for Supercomputing Applications)</td>
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<tr>
<td>10:00 am</td>
<td>Grand Ballrooms Foyer</td>
<td>BREAK</td>
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<tr>
<td>10:15 am</td>
<td>Grand Stations III &amp; IV</td>
<td>Science Track</td>
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<td></td>
<td>Session chair: Jay Alameda, Yang Wang</td>
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<tr>
<td>10:15 am</td>
<td>Brighton I-V Technology</td>
<td>Technology Track</td>
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<td>Session chair: Stephen McNally</td>
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<tr>
<td>10:15 am</td>
<td>Grand Station V</td>
<td>Gateways Track</td>
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<td></td>
<td></td>
<td>Session chair: Matthew Woitaszek</td>
</tr>
<tr>
<td>10:15 am</td>
<td>Biomolecular Simulations</td>
<td>Jeffrey Madura, Eliana Asciutto, Bonnie Merchant</td>
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<tr>
<td>10:45 am</td>
<td>UltraScan: High-resolution modeling of analytical ultracentrifugation experiments on TeraGrid</td>
<td>Emre Brookes, Borries Demeler</td>
</tr>
<tr>
<td>11:15 am</td>
<td>Numerical Simulations of Coupled Electro-Mechanical Dynamics in a Dog Ventricle</td>
<td>Henian Xia, Kwai Wong, Wenjun Ying, Xiaopeng Zhao</td>
</tr>
<tr>
<td>11:45 am</td>
<td>PLSQR: An MPI based Parallel Implementation of LSQR Algorithm for Seismic Tomography</td>
<td>He Huang, Liqiang Wang</td>
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<tr>
<td>12:15 pm</td>
<td>Reflections, Waterfront</td>
<td>BOX LUNCH</td>
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Tutorials

How to Design a Cluster that Works with the TeraGrid
Monday, 8 am – 12 pm | Grand Station II
Daniel LaPine, Jeremy Enos, Nathaniel Mendoza

Introduction to Scientific Visualization on Longhorn
Monday, 8 am – 12 pm | Grand Station III
Kelly Gaither

Running Applications at Scale on the First Academic Petaflop Supercomputer (full day)
Monday, 8 am – 5 pm | Grand Station IV
Glenn Brook, Lonnie Crosby, Meng-Shiou Wu, Haihang You

Cloud Technologies, Data-Intensive Science and the TeraGrid
Monday, 8 am – 12 pm | Grand Station V
Scott McCaulay, Judy Qiu, Marlon Pierce, Rich Knepper

Building Science Gateway Applications
Monday, 8 am – 12 pm | Ellwood
Yan Liu, Shaowen Wang, Nancy Wilkins-Diehr

HPC Applications Best Practices
HPC Advisory Council Tutorial
Monday, 8 am – 12 pm | Haselton
Gilad Shainer, Tong Liu, David Cownie, Jeff Layton

Optimization in Multi-Core Systems
Monday, 8 am – 12 pm | Brighton I
Kent Milfeld, Lars Koesterke, Carlos Rosales

Parallel Simulations and Science Gateways on the MATLAB Resource at Cornell
Monday, 8 am – 12 pm | Brighton II
Nathaniel Woody, Susan Mehringer, Steven Clark

Computing Across Both Open Science Grid and the TeraGrid
Monday, 1 pm – 5 pm | Grand Station II
John McGee, Mats Rynge, Jason Reilly

Introducing RDAV & Nautilus for Visualization, Data Analysis and Workflows
Monday, 1 pm – 5 pm | Grand Station III
Sean Ahern, Gary Liu, Amy Szczepanski, Scott Zimmerman

Open Grid Environments Software for Science Gateways
Monday, 1 pm – 5 pm | Grand Station V
Marlon Pierce, Suresh Marru

Performance Analysis and Tuning for GPUs
Monday, 1 pm – 5 pm | Ellwood
Richard Vuduc, Hyesoon Kimy, Brandon Hill, Tabitha Samuel

PerfExpert: An Automated Approach to Analyzing and Optimizing the Node-Level Performance of HPC Applications
Monday, 1 pm – 5 pm | Haselton
James Browne, Martin Burtscher,

vSMP and Flash Technologies for Data-Intensive Applications
Monday, 1 pm – 5 pm | Brighton I
Mahidhar Tatineni, Jerry Greenberg, Arun S. Jagatheesan

Scalable Systems Management with Puppet
Monday, 1 pm – 5 pm | Brighton II
Stephen McNally, Nick Jones

Birds of a Feather

TeraGrid’10 BOFs will engage attendees in exciting, informal, interactive sessions devoted to forward-looking topics drawn from the areas described in the submission guidelines for the Science, Technology, Gateways, and EOT tracks.

New Compute Systems in the TeraGrid Pipeline
Leader: Richard Moore

“MATLAB on the TeraGrid” Experimental Resource: Information, Getting Started, and Success Stories
Leader: David Lifka

Data Curation and Management in the TeraGrid
Leaders: Chris Jordan, J Ray Scott, Stephen Simms

Extending Cyberinfrastructure Beyond Its Own Boundaries -- Campus Champion Program
Leader: Kay Hunt

Common User Environments Working Group - Progress Report of Users
Leader: Shawn Brown

SLASH2: Next Generation Filesystem for Cooperating Scientific Institutions
Leaders: Paul Nowoczynski, Jared Yanovich, Zhihui Zhang

NSF DataNet Program Overview and Community Input Solicitation
Leaders: Philip Bogden, William Michener, Sayeed Choudhury, John Cobb, Tim DiLauro
**Visualization Showcase**
The Visualization Showcase provides a digital gallery of the powerful, evocative imagery associated with TeraGrid’s most exciting and compelling results. Featured projects have used TeraGrid resources to generate data, to produce the visualization, or both, and are the result of work accomplished within the past year.

1. **Chino Hills - A Highly Computationally Efficient Earthquake Simulation**  
   **Greg Foss, Jacobo Bielak, Ricardo Taborda, Haydar Karaoglu**

2. **GlyphSea**  
   **Amit Chourasia, Emmett Mcquinn, Bernard Minster, Jurgen Schulze**

3. **Visualization of Tiger Simulation**  
   **Amit Chourasia, Renyue Cen**

4. **Large-scale volumetric visualization of Doppler reflectivity data**  
   **Peter Kristof, Jin Ryong Kim, Bedrich Benes, Lan Zhao, Carol X. Song**

5. **Searching for Baryon Acoustic Oscillations in Intergalactic Absorption, Project StarGate Application Driver**  
   **Micheal Norman, Robert Harkness, Pascal Paschos, Rick Wagner, Mark Hereld, Joseph Insley, Eric Olson, Michael Papka**

6. **Ozone Concentrations in Eastern Texas Due to Emissions in Houston**  
   **Gregory P. Johnson**

7. **Searching for Baryon Acoustic Oscillations in Intergalactic Absorption, The Expanding Universe**  
   **Micheal Norman, Robert Harkness, Pascal Paschos, Rick Wagner, Mark Hereld, Joseph Insley, Eric Olson, Michael Papka**

8. **Visualization of Large Electronic Records Collection**  
   **Maria Esteva, Suyog D Jain, Weijia Xu**

9. **Web Based Visualization using TACC’s Longhorn Visualization Portal and Envision**  
   **Brandt Westing**

10. **Selections from Violent Storm Simulation**  
    Animations shown at the workshop Data Visualization: Taking the Presentation of Methods and Results to the Next Level, Imiloa Astronomy Center, Hilo, Hawai‘i, 2009  
    **Greg Foss, Ming Xue, Jili Dong, Christopher Phillips, David O’Neal**

**Special Presentations**

**TeraGrid Overview**
Tuesday, 8:30 am (preceding the keynote) | Grand Station I-V  
**Speaker:** John Towns, National Center for Supercomputing Applications  
A brief overview of TeraGrid activities during 2009/2010, including the latest metrics on the infrastructure’s resources, usage, and users.

**Panel Session: Advanced Cyberinfrastructure Integration with Large Scale NSF Science and Engineering Projects**
Tuesday, 1:15 pm | Grand Station I-II  
**Moderator:** John Cobb, Oak Ridge National Laboratory  
Panelists will describe several large-scale NSF science and engineering projects that make integrated use of advanced cyberinfrastructure. Further discussion will include insights on how best to utilize (common) cyberinfrastructure to advance science and opportunities for future “eXtreme Digital” (XD) activities to build upon these efforts.

Panelists: Kent Blackburn (LIGO), Barb Fossum (NEES), John Orcutt (OOI), Dan Stanzione (iPlant)

**The Transition from TeraGrid to XD**
Wednesday, 8:30 am (preceding the keynote) | Grand Station I-V  
**Speaker:** Richard Moore, San Diego Supercomputer Center  
A brief summary of activities as the current TeraGrid program transitions to the next-generation eXtreme Digital (XD) program in 2011, with focus on impacts to the user community.

**Plenary Session (Part 1): Technology Audit and Insertion Services**
Wednesday, 1:15 pm | Grand Station I-II  
**Session Chair:** Richard Moore, San Diego Supercomputer Center  
Overview and discussion of these two new awards from the National Science Foundation, initiating the rollout of the “eXtreme Digital” (XD) program.

Participants: Tom Furlani, Director of the University at Buffalo’s Center for Computational Research (CCR) and Principal Investigator, Technology Audit Service; John Towns, Director of the Persistent Infrastructure Directorate, National Center for Supercomputing Applications, and Principal Investigator, Technology Insertion Service.

**Plenary Session (Part 2): Enabling Discovery with Dell HPC Solutions on the TeraGrid** (Sponsor Presentation)  
**Speaker:** Jim Gutowski, HPC Business Development Manager for Research Computing, Dell  
Dell collaborates with many TeraGrid institutions which provide and consume high-performance computing resources. This presentation focuses on enabling research and scientific discovery through the implementation of Dell HPC solutions as TeraGrid resources, including clusters at NCSA, TACC, and Cornell.

TeraGrid wishes to thank Dell as a Gold sponsor for TG’10.
Posters and Demos

The TeraGrid ‘10 Poster Session and Reception will be from 7 to 9 p.m. on Tuesday, August 3 in Admiral, Reflections, and Waterfront. Work submitted to the Poster Track and the Student Program will be presented, with awards given for the best posters.

1. A Comparative Analysis of Localized Command Line Execution, Remote Execution through Command Line, and Torque Submissions of MATLAB Scripts for the Charting of CReSIS Flight Path Data
   Robyn Evans and JerNettie Burney, Elizabeth City State University

2. Simulation of Bone-conducted Sound Pathways to the Outer and Middle Ear
   Margaret Wismer, University of Illinois

3. Membrane-Solvated Molecular Dynamics on Neurotransmitter Transporter Homology Models Using the TeraGrid
   Michael Braden, University of Montana

4. A Computational Approach to Knotting in Complete Graphs
   Dana Rowland and David Toth (presenting), Merrimack College

5. Computational Investigation of Four Valence Electron Silicon Reactive Intermediates
   Sophia White and Peter P. Gaspar, Washington University

6. Parallel Implementation and Code Development of Efficient Multibody Algorithm for Motion Simulation of Molecular Structures on TeraGrid Supercomputers
   Wen Duan, University of California at Berkeley; Shanzhong Duan, South Dakota State University

7. The Effect of Interaction with Silica Surface on the Conformation of Antimicrobial Peptide Cecropin P1C Using Molecular Dynamics Simulation
   Hector Chang, Ganesan Narsimhan and Xiaoyu Wu, Purdue University

8. Benchmark Solutions for the Incompressible Navier-Stokes Equations Using a Parallel Consistent Splitting Scheme
   Mikhail Sekachev and Kwai Wong, University of Tennessee

9. Efficient Algorithm for Virtual Prototyping of Large-Sized Multibody Dynamical Systems on TeraGrid
   Shawn Duan and Abdul Muqtadir Mohammed, South Dakota State University

10. Mentoring Minority Undergraduates in their Efforts to Implement a LAMP Documentation Server for a Condor-based Grid
    Linda Hayden, Jeaine Powell, Elizabeth City State University; Felicia Doswell, Norfolk State University; and Kaiem Frink, Elizabeth City State University

11. Pegasus WMS - Bridging the National CyberInfrastructure Divide to Run Large Scale Scientific Workflows
    Gaurang Mehta, Ewa Deelman, Karan Yahi, Gideon Juve, Philip Maechling, Thomas Jordan, Scott Callaghan, University of Southern California; Miron Livny and Kent Wenger, University of Wisconsin Madison

    Mats Rynge, Ewa Deelman, Gideon Juve, University of Southern California; Burt Holzman, Krista Larson, Fermi Laboratory; Frank Wuerthwein and Igor Sfiligoi, University of California at San Diego

    Igor Sfiligoi, Frank Wuerthwein and Christopher Theissen, University of California at San Diego

14. A Parallel Agent Based Model to Describe Host-Pathogen Interaction for Toxoplasma Gondii
    Adam Sullivan, Kwai Wong, Chunlei Su and Xiaopeng Zhao, University of Tennessee

15. Space Radiation Estimation and Prediction on TeraGrid
    Liwen Shih, University of Houston at Clear Lake

16. Multi-scaled Properties Simulation of Carbon Nanofiber Reinforced Space Polymer Composites
    Li Sun, University of Houston; Liwen Shih, University of Houston at Clear Lake

17. Konfuse - Kerberos Over the Network via FUSE
    Robert Budden, Josephine Palencia and Paul Nowoczenski, Pittsburgh Supercomputing Center

18. Sky Computing on FutureGrid and Grid’5000
    Pierre Riteau, Université de Rennes; Mauricio Tsugawa, Andrea Matsunaga, José Fortes, University of Florida; Kate Keahey, Argonne National Laboratory

19. Comprehensive File Management in the TeraGrid
    Rion Dooley, Maytal Dahan, Matthew Hanlon, Stephen Mock and Praveen Nuthulapati, Texas Advanced Computing Center

20. LEAD II: Hybrid Workflows in Atmospheric Science
    Beth Plade, Indiana University; Craig Mattocks, University of North Carolina at Chapel Hill; Keith Brewster, University of Oklahoma; Eran Chinshaka, Jeff Cox, Chathura Herath, Scott Jensen, Yuan Lao, Yiming Sun, Felix Terkhorn, (presenting), Ashish Bhangle, Kavitha Chandrasekar, Prashant Sabhnani, Robert Ping, Indiana University
1. A Comparison of Job Duration Utilizing High Performance Computing on a Distributed Grid
Jernettie Burney and Michael Austin

2. Interactive Visualization of Multi-Terabyte Cosmological Data Sets
Joshua Tepper

3. Entropy of Octagonal Tiling Representations of Quasicrystals
Maxwell Hutchinson

4. A Dynamic Agent-Based Data Distribution Framework
Andrew Pfeifer

5. Analyzing Projected Changes and Trends of Temperature and Precipitation in SCIPP Area from Sixteen Downscaled Global Climate Models under Different Emission Scenarios
Lu Liu

6. A Hybrid MPI and GPU Approach to Efficiently Solving for Solving Large-sized kNN Problems
Libin Sun, Cyrus Stoller and Tia Newhall

7. Parallel Simulation and Virtual Prototyping of Multi-body Dynamical Systems on TeraGrid Supercomputers
Abdul Muqtadir Mohammed and Shawn Duan

8. Stability of Networked Feedback Control Systems under Quantization
Laurentiu Marinovici

9. Calculating Activation Pathways of Adenovirus Protease Enzymes using the AMBER Molecular Dynamics Package on TeraGrid Resources
Parastou Sadatmousavi and Ross Walker

10. Waste Water Utilization into Transportation
Rijan Karke

11. A Computational Approach to Ramsey Theory
Stephan Krach, David Toth and Michael Bradley

12. Parallel Implementation and Code Development of Efficient Multibody Algorithm for Motion Simulation of Molecular Structures on TeraGrid Supercomputers
Wen Duan and Shanzhong Duan

13. Tool for Visual Comparison of Massive Data Sets Through Aggregation Techniques
Hooman Hemmati, Duber Gomez Fonseca and Sarah Jennisca

14. Practical Investigations for Task-Parallel Programming
Robert Dunn Jr. and Hongmei Chi

15. Molecular Modeling Scheme to Efficiently Determine the Selectivity of Various Calix-Crown Molecules with Cs, K, and Na Ions
Steven Baker, B. Ramu and P. Derosa

16. Using a Regional Climate Model to Simulate Heavy Precipitation Events in Central Illinois
Wenjing Jia, Don Wuebbles and Xin-Zhong Liang

17. Automated System To Construct A Simulated Hurricane Database
Swathi Laxmi Dubbaka, Ram Sri Harsha Bhagawaty, Lei Jiang, Kelin Hu, Sreekanth Pathanis, Nathan Brener, Erik Schnetter, Gabrielle Allen, S. Sitharama Iyengar and Tevfik Kasar

18. Lightweight OGCE Gadget Portal for Science Gateways
Zhenhua Guo and Marlon Pierce

19. Simplifying Complex Software Assembly: The Component Retrieval Language and Implementation
Eric Seidel, Gabrielle Allen, Steven Brandt, Frank Löffler and Erik Schnetter

20. Simulation Factory: Simplified Simulation Management
Michael Thomas, Erik Schnetter and Gabrielle Allen

21. Toward A Parallel Spatially-Explicit Agent-Based Modeling Framework
Eric Shook, Shaowen Wang and Wenwu Tang

22. Recreating Drama in the Delta Using 3D Modelling and Animation
Michelle Chen, Amit Chourasia, Emily Roxworthy and Leonel Lopez

23. Application-Level Debugging and Runtime Visualization Tools for Parallel Simulations within the Cactus/Carpet Framework
Oleg Karabkin, Eloisa Bentivegna and Erik Schnetter

24. Intelligent Application-Level Task Migration
Ashley Zebrowski, Gabrielle Allen and Peter Diener

25. An OpenMP Overdrive for LAMMPS - Improving MD Performance on the TeraGrid Through Hybrid OpenMP/MPI Parallelization
Peter Shannon, Ryan Houlihan and Axel Kohlmeyer

26. Role of Diffusion in Scaling of Polymer Chain Aggregates Found in Chemical Vapor Deposition Growth Model
Sairam Tangirala and David P. Landau
The TG’10 committee wishes to thank our sponsors for their generous support!

Help us make TeraGrid’11 even better!
Share your perspective on this year’s TeraGrid conference.
Following the conference on Thursday, August 5, please fill out the brief evaluation form at:

http://www.teragrid.org/tg10/evaluation